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Photodissociation Dynamics of Cluster Ions

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Michael T. Bowers

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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

Progress has been Made on the Following Two Objectives:

- 1) Photodissociation Dynamics of Small Cluster Ions
(11 papers on 8 different clusters)
- 2) Generation, Structure and Reactivity of Metallic and Semiconductor Clusters
(7 papers on various aspects)

A new technique for obtaining the structure of gas phase clusters was developed

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22a. NAME OF RESPONSIBLE INDIVIDUAL

Dr. Michael Berman

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AFOSR Grant 89-0102

Photodissociation Dynamics of Cluster Ions
Final Report

November 15, 1988 to November 14, 1991

I. Abstract

There are two somewhat different objectives of this grant, unified by their common interest in clusters. We have made substantial progress both in photodissociation of atmospheric clusters (11 papers) and in the generation and reactivity of semiconductor and metallic clusters (7 papers). Of particular interest is our development of a new "ion chromatography" technique that allows determination of the shape of clusters, or other species, in the gas phase.

II. Objectives

- A. Photodissociation Dynamics of Atmospheric Cluster Ions
- B. Generation, Structures and Reactivity of Semiconductor and Metallic Cluster Ions

III. Progress

A. Photodissociation Dynamics of Cluster Ions

The progress made in this area has been described in detail in the two progress reports, the proposal funded as a one year extension to AFOSR 89-0102, and the proposal that recently was approved for funding commencing November 15, 1992. Consequently, only a list of the systems completed will be given here, with the associated papers tabulated in the publications section: Ar_3^+ (2 papers), CO_3^- , $(\text{C}_6\text{H}_6)_2^+$, $(\text{S}\cdot\text{SO}_2)^+$, $(\text{Ar}\cdot\text{N}_2)^+$, $\text{Kr}\cdot\text{H}_2\text{O}^+$, $\text{CO}_3^-\cdot\text{H}_2\text{O}$ and $(\text{OCS}\cdot\text{C}_2\text{H}_2)^+$.

B. Carbon Clusters

Again, the work accomplished has been discussed in detail in the interim reports and proposals on file. The most important aspect of this work is the use of our recently developed "ion chromatography" technique for studying structures of carbon cluster ions.

C. Reactions of Transition Metal Cluster Ions

During the review period we were able to develop methods for generating intense beams of mass selected cluster ions up to M_{20}^+ for $\text{M} = \text{Nb}, \text{Co}$.

Preliminary reactions studies indicate this will be a fruitful area of research in the future.

IV. Papers published or in Press

1. Photodissociation Dynamics of $C_4H_6^+$ Ions from 1,3-Butadiene, T. Bunn and M.T. Bowers, *J. Phys. Chem.* **92**, 1813 (1988).
2. Photodissociation Dynamics of Small Cluster Ions, M.T. Bowers in *Ion and Cluster Ion Spectroscopy and Structure*, J.P. Maier (Ed.), Elsevier, Amsterdam, pp. 241-275 (1989).
3. Structure, Reactivity and Energetics of Covalently Bound Carbon Cluster Ions, C_5^+ to C_{11}^+ : Experiment and Theory, P. Radi, M.E. Rincon, M.T. Hsu, J. Brodbelt-Lustig, P. Kemper and M.T. Bowers, *J. Phys. Chem.* **93**, 6187 (1989).
4. Photodissociation Dynamics of Ar_3^+ , J.T. Snodgrass, C.M. Roehl and M.T. Bowers, *Chem. Phys. Lett.* **159**, 10 (1989).
5. Photodissociation of CO_3^- in the Gas Phase: Product Kinetic Energy Measurements as a Probe of Excited State Potential Surfaces and Dissociation Dynamics, J.T. Snodgrass, C.M. Roehl, P.A.M. van Koppen, W. Palke and M.T. Bowers, *J. Chem. Phys.* **92**, 5935 (1990).
6. Photodissociation of the Benzene Dimer Cation in the Gas Phase, J.T. Snodgrass, R.C. Dunbar and M.T. Bowers, *J. Phys. Chem.* **94**, 3648 (1990).
7. The Mechanism and Photodissociation Dynamics of the $(S \cdot SO_2)^+$ Cluster at 308 nm, J.T. Snodgrass, T.L. Bunn and M.T. Bowers, *Int. J. Mass Spectrom. Ion Proc.* **102**, 45 (1990) (Special Issue on Clusters).
8. Evaporation of Covalent Clusters: Unimolecular Decay of Energized Size Selected Carbon Cluster Ions (C_n^+ , $5 \leq n \leq 100$), P.P. Radi, M.T. Hsu, J. Brodbelt-Lustig, M. Rincon and M.T. Bowers, *J. Chem. Phys.* **92**, 4817 (1990).
9. Energetics, Structure and Photodissociation Dynamics of the Cluster $Ar \cdot N_2^+$, H-S. Kim and M.T. Bowers, *J. Chem. Phys.* **93**, 1158 (1990).
10. Observation of Small Doubly Charged Niobium Clusters, P.P. Radi, G. von Helden, M-T. Hsu, P.R. Kemper and M.T. Bowers, *Chem. Phys. Lett.* **179**, 531 (1991).
11. Photodissociation Dynamics of Water Containing Clusters: $Kr \cdot H_2O^+$, H-S. Kim, C-H. Kuo and M.T. Bowers, *J. Chem. Phys.* **93**, 5594 (1990).
12. On the Structure, Reactivity and Relative Stability of the Large Carbon Cluster Ions C_{62}^+ , C_{60}^+ and C_{58}^+ , P.P. Radi, M.-T. Hsu, M.E. Rincon, P.R. Kemper and M.T. Bowers, *Chem. Phys. Lett.* **174**, 223 (1990).
13. Reply to the Comment on Evaporation of Covalent Clusters: Unimolecular

- Decay of Energized Size Selected Carbon Clusters, M.T. Bowers, P.P. Radi and M.-T. Hsu, *J. Chem. Phys.* **95**, 3835 (1991).
14. Photodissociation of $\text{CO}_3^-\bullet\text{H}_2\text{O}$: Observation of the $\text{O}^-\bullet\text{H}_2\text{O} + \text{CO}_2$ Product Channel, C.M. Roehl, J.T. Snodgrass and M.T. Bowers, *J. Chem. Phys.* **94**, 6546 (1991).
 15. Thermal Bimolecular Reactions of Size Selected Transition Metal Cluster Ions: $\text{Nb}_n^+ + \text{O}_2$, $n = 1$ to 6, P.P. Radi, G. von Helden, M.-T. Hsu, P.R. Kemper and M.T. Bowers, *Int. J. Mass Spectrom. Ion Proc.*, Paul Kebarle Honor Issue **109**, 49 (1991).
 16. On the Structure and Photodissociation Dynamics of Ar_3^+ , M.T. Bowers, W.E. Palke, K. Robbins, C. Roehl and S. Walsh, *Chem. Phys. Lett.* **180**, 235 (1991).
 17. The Dynamics of Metastable Dissociation and Photodissociation of the Gas Phase Cluster Ion $(\text{OCS}:\text{C}_2\text{H}_2)^+$, S.T. Graul and M.T. Bowers, *J. Phys. Chem.* **95**, 3828 (1991).
 18. Structures of Carbon Cluster Ions from 3 to 60 Atoms: Linears to Rings to Fullerenes, G. von Helden, M.-T. Hsu, P.R. Kemper and M.T. Bowers, *J. Chem. Phys.* **95**, 3895 (1991).

V. Personnel Associated with the Project

A. Senior

Dr. Paul Kemper	Dr. Chou-Hong Kuo
Dr. Peter Radi	Dr. Joe Snodgrass
Dr. Susan Graul	Dr. Tom Bunn
Dr. Jennifer Brodbelt	Dr. Petra van Koppen

B. Junior

Ms. Hyun-Sook Kim	Ms. Coleen Roehl
Mr. Gert von Helden	Mr. Ming-Teh Hsu
Ms. Marina Rincon	Ms. Kathy Robbins
Ms. Sherrie Walsh	

VI. Papers Presented at Meetings/Universities

A. Invited Lectures

1. Award Lecture, Nobel Laureate Signature Award Symposium, 198th National Meeting of the American Chemical Society, Miami, FL, September 1989.
2. Invited Lecturer (two lectures), NATO Advanced Study Institute on Fundamentals of Gas Phase Ion Chemistry, Mont. Ste. Odile, France, July 1990 (Carbon and Metal Clusters).

3. Invited Speaker, Gordon Research Conference on Molecular and Ionic Clusters, Volterra, Italy, September 1990 (Photodissociation Dynamics of Small Cluster Ions).
4. Invited Speaker, 8th Asilomar Conference on Reaction Intermediates, Pacific Grove, CA, September 1990 (Ion Chromatography and Metallic Clusters).
5. Invited Lecturer, Sanibel Conference on Chemical Activation, Sanibel Island, FL, January 1991 (Photodissociation Dynamics of Small Clusters).
6. Invited Speaker, Gordon Conference on the Structure, Energetics and Reaction Dynamics of Gaseous Ions, Ventura, CA, March 1991 (Ion Chromatography).
7. Invited Lecturer, Symposium on Reactions, Spectroscopy and Structure of Molecular Ions, 199th National American Chemical Society Meeting, Atlanta, GA, April 1991 (Ion Chromatography).
8. Invited Lecturer, Franklin and Field Award Symposium, 199th National American Chemical Society Meeting, Atlanta, GA, April 1991 (Carbon Clusters).
9. Invited Lecturer, Workshop on the Activation and Dissociation of Big Ions, Battelle Northwest Conference Center, Seattle, WA, May 1991 (Ion Chromatography and Photoactivation).

B. Contributed Papers at Conferences (Topics not given for sake of brevity)

1. Presented two papers at the Informal Conference on Photochemistry, Santa Monica, CA, January 1989.
2. Presented four papers, Western Regional Conference on Ion Chemistry, Lake Arrowhead, CA, February 1989.
3. Presented four papers, American Society for Mass Spectrometry National Meeting, Miami, FL, May 1989.
4. Presented Paper at Faraday Symposium 25: Large Gas Phase Clusters, Warwick University, Coventry, United Kingdom, December 1989.
5. Presented poster, AFOSR Meeting on High Energy Density Materials, Long Beach, CA, February 1990.
6. Presented four papers, Western Regional Conference on Ion Chemistry, Lake Arrowhead, CA, February 1990.
7. Presented three papers, American Society for Mass Spectrometry National Meeting, Tucson, AZ, June 1990.
8. Presented three papers, 12th International Conference on Mass

Spectrometry, Amsterdam, The Netherlands, August 1991.

C. Invited Seminars at Universities

1. Iowa State University, Ames, IA, February 1989.
2. University of California, Los Angeles, CA, February 1989.
3. University of California, Santa Cruz, CA, March 1990.
4. University of Texas, Austin, TX, October 1990.
5. Rice University, Houston, TX, October 1990.
6. University of Southern California, Los Angeles, CA, November 1990
7. University of Utah, Salt Lake City, UT, May 1991.
8. University of Sussex, Brighton, United Kingdom, September 1991
9. University of Warwick, Coventry, United Kingdom, September 1991
10. Texas A&M University, College Station, TX, October 1991
11. University of Texas at Arlington, TX, October 1991.
12. University of California, San Diego, CA, November 1991
13. California Institute of Technology, Pasadena, CA, November 1991

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